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Journal of Computational and Applied Mathematics 199 (2007) 207–212

JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

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Reduction of overestimation in interval arithmetic simulation of biological wastewater treatment processes

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Received 2 December 2004

Abstract

A novel interval arithmetic simulation approach is introduced in order to evaluate the performance of biological wastewater treatment processes. Such processes are typically modeled as dynamical systems where the reaction kinetics appears as additive nonlinearity in state. In the calculation of guaranteed bounds of state variables uncertain parameters and uncertain initial conditions are considered. The recursive evaluation of such systems of nonlinear state equations yields overestimation of the state variables that is accumulating over the simulation time. To cope with this wrapping effect, innovative splitting and merging criteria based on a recursive uncertain linear transformation of the state variables are discussed. Additionally, re-approximation strategies for regions in the state space calculated by interval arithmetic techniques using disjoint subintervals improve the simulation quality significantly if these regions are described by several overlapping subintervals. This simulation approach is used to find a practical compromise between computational effort and simulation quality. It is pointed out how these splitting and merging algorithms can be combined with other methods that aim at the reduction of overestimation by applying consistency techniques. Simulation results are presented for a simplified reduced-order model of the reduction of organic matter in the activated sludge process of biological wastewater treatment.

Keywords: Uncertain nonlinear systems; Interval arithmetics; Wastewater treatment; Guaranteed simulation; Wrapping effect

1. Introduction

Analysis, control, and optimization of wastewater treatment processes are important tasks in bioprocess engineering, not only for economic reasons but also for reduction of environmental problems caused by water pollution. Modern wastewater treatment plants are complex biochemical systems. Biological wastewater treatment processes are characterized by additive nonlinear kinetics describing the growth rates of bacteria which are responsible for purification. Moreover, most system parameters and initial states are uncertain. Expert knowledge about the system dynamics allows to specify guaranteed worst-case bounds of all system parameters. To prove correct operation of wastewater treatment plants such that they meet international regulations and to analyze their performance with respect to parameter variations, appropriate simulation techniques have to be applied. Since grid-based or stochastic simulation techniques, e.g. Monte Carlo methods, in general, cannot provide guaranteed bounds of the system states, interval techniques are

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doi:10.1016/j.cam.2005.07.029

applied in this paper [3,5]. Reduction of the wrapping effect and other sources of overestimation are addressed to determine tight interval enclosures of all state variables. In Section 2, a detailed description of a reduced-order system model in biological wastewater treatment is given [6]. In Section 3, a pseudo-linear recursive uncertain transformation of the set of state equations is introduced. An overview of the proposed interval algorithm is presented in Section 4. Splitting and merging strategies of subintervals as well as simulation results for the subsystem of biological wastewater treatment are presented in Section 5. In Section 6, conclusions and an outlook on future research are given.

2. System modeling of biological wastewater treatment processes

Modern biological wastewater treatment plants consist of several activated sludge tanks (aeration tanks) and settler tanks [1]. A simple block diagram of such systems is depicted in Fig. 1. The inflow of wastewater is Q_{W} with external oxygen supply u_{O_2} into the aeration tank.

In this paper, only the reduction of biodegradable organic matter (substrate concentration S) by heterotrophic bacteria (concentration X) is considered with the oxygen concentration S_{O} in the aeration tank. In the settler model, a perfect separation of clean wastewater (flow $Q_{\mathrm{W}} - Q_{\mathrm{EX}}$) and activated sludge is assumed. This sludge is fed back partially into the aeration tank (Q_{RS}) while the remaining excess sludge Q_{EX} is removed from the process. The bacteria concentration in the settler is denoted by X_{Set}. According to the Activated Sludge Model ASM1 of the International Association on Water Quality biological wastewater treatment processes can be described by coupled nonlinear differential equations. Most system parameters are uncertain because of disturbances in composition and amount of the influent wastewater as well as changing temperature and weather conditions. The reduction of biodegradable organic matter is thus described by four differential equations [6]

$$\begin{aligned}
\dot{S} &= \frac{Q_{\mathrm{W}}}{V_{\mathrm{A}}}(S_{\mathrm{W}} - S) - \mu(S, S_{\mathrm{O}})\frac{1}{Y}X,\\
\dot{X} &= -\frac{Q_{\mathrm{W}}}{V_{\mathrm{A}}}X + \frac{Q_{\mathrm{RS}}}{V_{\mathrm{A}}}(X_{\mathrm{Set}} - X) + (\mu(S, S_{\mathrm{O}}) - b)X,\\
\dot{S}_{\mathrm{O}} &= \frac{Q_{\mathrm{W}}}{V_{\mathrm{A}}}(S_{\mathrm{OW}} - S_{\mathrm{O}}) - \mu(S, S_{\mathrm{O}})\frac{1-Y}{Y}X + \frac{\rho_{\mathrm{O}_2}}{V_{\mathrm{A}}}\left(1 - \frac{S_{\mathrm{O}}}{S_{\mathrm{O,sat}}}\right)u_{\mathrm{O}_2},\\
\dot{X}_{\mathrm{Set}} &= \frac{Q_{\mathrm{W}} + Q_{\mathrm{RS}}}{V_{\mathrm{Set}}}X - \frac{Q_{\mathrm{EX}} + Q_{\mathrm{RS}}}{V_{\mathrm{Set}}}X_{\mathrm{Set}},
\end{aligned} \tag{1}$$

with a nonlinear growth rate of substrate consuming bacteria modeled by the Monod kinetics

$$\mu(S, S_{\mathrm{O}}) = \hat{\mu}_{\mathrm{H}}\frac{S}{S + K_{\mathrm{S}}}\frac{S_{\mathrm{O}}}{S_{\mathrm{O}} + K_{\mathrm{OS}}}. \tag{2}$$

The nominal system parameters are summarized in Table 1. All interval simulations presented in this paper assume an uncertainty of $\pm 10\%$ of the maximum specific growth rate $\hat{\mu}_{\mathrm{H}}$ which may be time-varying arbitrarily between the infimum and supremum of its range. The set of state equations (1) is abbreviated by $\dot{x} = f(x(t), p(t))$ which is discretized for simulation purposes by the explicit Euler method $x_{k+1} = x_k + Tf(x_k, p_k)$ with $T = 40\,\mathrm{s} = \mathrm{const}$, where all state variables are summarized in the vector $x = [S; X; S_{\mathrm{O}}; X_{\mathrm{Set}}]^{\mathrm{T}}$. The discretization error is neglected in this paper. However, it can be considered easily in the suggested approach, see e.g. [2].

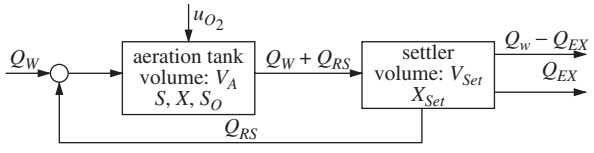

Fig. 1. Block diagram of a simplified biological wastewater treatment process.

Table 1
Nominal values of the system parameters

Parameter	Nominal value
V_A: volume of the aeration tank	$8000\,m^3$
V_{Set}: volume of the settler	$4545\,m^3$
Q_W: influent wastewater flow rate	$0.153\,m^3/s$
Q_{RS}: flow rate of return sludge	$0.0916\,m^3/s$
Q_{EX}: flow rate of excess sludge	$0.005\,m^3/s$
S_W: influent biodegradable substrate concentration	$0.616\,kg/m^3$
S_{OW}: influent oxygen concentration in the wastewater	$0.5 \cdot 10^{-3}\,kg/m^3$
$S_{O,sat}$: saturation concentration of dissolved oxygen	$5.3 \cdot 10^{-3}\,kg/m^3$
Y: yield coefficient of heterotrophic biomass	0.67
$\hat{\mu}_H$: max. specific growth rate of heterotrophic biomass	$1/14400\,1/s$
b: specific decay rate of heterotrophic biomass	$7.176 \cdot 10^{-6}\,1/s$
K_S: half saturation coefficient for heterotrophic biomass	$0.02\,kg/m^3$
K_{OS}: oxygen half saturation coefficient	$2 \cdot 10^{-4}\,kg/m^3$
u_{O_2}: influent oxygen flow rate (constant)	$1.487\,m^3/s$
ρ_{O_2}: normal density of molecular oxygen	$1.428\,kg/m^3$

3. Pseudo-linear transformation of state equations

In interval simulations the wrapping effect arises if non-axis-parallel regions in the state space are replaced by axis-parallel enclosures in each simulation step. This is shown for a linear state equation $x_{k+1} = \mathbf{A}x_k$, where $\mathbf{A}$ is a rotation matrix of 45° and the initial state interval $x_0 = [[-1; 1]; [-1; 1]]^T$, see first row of Fig. 2. If in recursive evaluation of the state equation according to $x_{k+1} = \mathbf{A}\tilde{\mathbf{A}}_{k-1}\ x_0 = \tilde{\mathbf{A}}_k x_0$ with $k \geqslant 0$ and $\tilde{\mathbf{A}}_{-1} = \mathbf{I}$ all state intervals x_{k+1} are related directly to the initial interval x_0 by $\tilde{\mathbf{A}}_k$, the wrapping effect can be eliminated in this linear example (second row of Fig. 2), where the system matrix is a point matrix, see exact solution in the third row for comparison. The matrix $\mathbf{I}$ is an identity matrix of appropriate dimensions. Using this method for uncertain linear systems often leads to significant reduction of the wrapping effect. In the nonlinear system of biological wastewater treatment, rational nonlinearities in state have to be considered, where only the bacteria concentration $x_{\beta,k} = X$ does not appear in the denominator of the

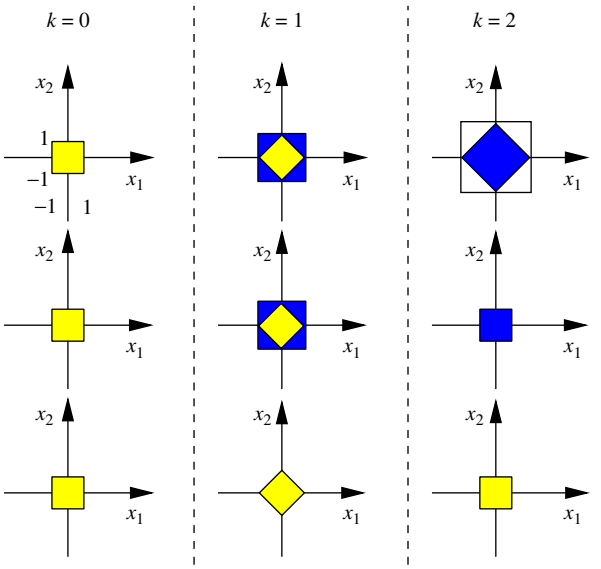

Fig. 2. Wrapping effect in interval simulation of discrete-time systems.

rational expression

$$r(x_k) = \left(\prod_{i=1}^{\alpha} \mu_i \, \frac{x_{i,k}}{x_{i,k} + K_i} \right) x_{\beta,k}; \quad \beta \notin \{1, \ldots, \alpha\}. \tag{3}$$

Defining an extended state vector $\tilde{x}_k = [x_k^{\mathrm{T}} \vdots 1]^{\mathrm{T}}$, the set of state equations is rewritten analytically in pseudo-linear form $\tilde{x}_{k+1} = \mathbf{A}_k(x_k) \cdot \tilde{x}_k$ after assigning the rational term in brackets in (3) to the state dependent matrix $\mathbf{A}_k(x_k)$. During simulation multiplication of the matrices $\tilde{\mathbf{A}}_k = \mathbf{A}_k(x_k)\tilde{\mathbf{A}}_{k-1}$ is performed recursively.

4. Interval simulation of uncertain discrete-time systems

In this section, the proposed interval algorithm for simulation of nonlinear discrete-time systems with uncertain parameters is discussed, see Fig. 3, where z^{-1} is the discrete-time unit-delay operator. Extensions of this algorithm to continuous-time problems are shown in [2]. To calculate tight enclosures of complex shaped regions in the state space, splitting of the initial list $L\{x_k\}$ in each time-step k into a list $L'\{x_k\}$ with more but smaller subintervals based on the introduced pseudo-linear transformation of state equations is performed. On one hand, the set of discrete-time state equations is evaluated using traditional interval methods including midpoint rule, monotonicity tests, and iterative optimization of infimum and supremum of the range of the state variables [4]. On the other hand, the state equations after pseudo-linear transformation are computed. Since both results $L'_1\{x_{k+1}\}$ and $L'_2\{x_{k+1}\}$ represent conservative state enclosures, intersection of corresponding interval boxes of both lists is allowed. Corresponding intervals that do not overlap are deleted from *both* lists.

After intersection only one list $L'\{x_{k+1}\}$ exists which can be checked for consistency with $L\{x_k\}$ as discussed in [2]. Afterwards, physical limitations of the state variables such as non-negativity of all concentrations as well as the saturation value $S_{\mathrm{O,sat}}$ of the oxygen concentration are taken into account. To provide a practical compromise between computational effort and simulation quality and to limit the number of subintervals, merging strategies are applied before the state equations are evaluated again in the following time-steps. The simulation quality is improved by re-approximation strategies which replace all subintervals by a new conservative approximation using disjoint interval boxes in case of a huge number of significantly overlapping subintervals.

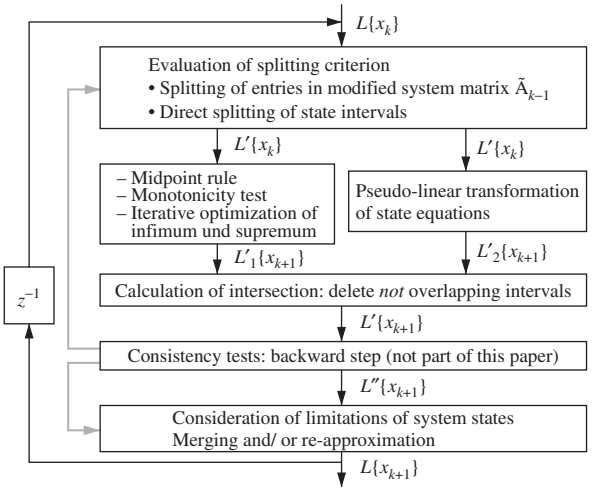

Fig. 3. Overview of proposed interval simulation algorithm.

5. Splitting and merging in simulation with several subintervals

In this section, basic splitting and merging strategies for interval simulations with several subintervals are summarized which reduce overestimation by improved approximation of complex shaped regions in the state space.

5.1. Splitting strategies

The basic idea of all splitting strategies is replacement of one interval box x_k by two interval boxes such that $\tilde{x}_k = \tilde{x}_{\alpha,k} \cup \tilde{x}_{\beta,k}$. After splitting the interval box x_k, the transformed state equations $\tilde{x}_{i,k+1} = \mathbf{A}_k(x_{i,k}) \cdot \tilde{x}_{i,k}$ are evaluated for both subintervals $i = \{\alpha, \beta\}$.

5.1.1. Direct splitting of state intervals

The first alternative for splitting of interval boxes is to divide one component of the interval vector x_k at its interval midpoint $\mathrm{mid}(x_{k,i})$, $i \in \{1, \ldots, n\}$. For example, splitting of the first component of a 2D state vector gives

$$x_{\alpha,k} = \begin{bmatrix} [\underline{x}_{k,1};\ \mathrm{mid}(x_{k,1})] \\ x_{k,2} \end{bmatrix} \quad \text{and} \quad x_{\beta,k} = \begin{bmatrix} [\mathrm{mid}(x_{k,1});\ \overline{x}_{k,1}] \\ x_{k,2} \end{bmatrix}. \tag{4}$$

The advantage of this procedure is that $\mathrm{int}\{x_{\alpha,k}\} \cap \mathrm{int}\{x_{\beta,k}\} = \emptyset$, where int denotes the interior of an interval. However, information about rotation of interval boxes in the state space stored in the modified system matrix is lost. Thereafter either $\tilde{x}_{i,k+1} = \mathbf{A}_k(x_{i,k})\mathrm{diag}(\tilde{x}_{\alpha,k})\tilde{x}_0^*$ with $\tilde{x}_0^* = [1 \ \ldots \ 1]^{\mathrm{T}}$ or $\tilde{x}_{i,k+1} = \mathbf{A}_k(x_{i,k}) \cdot \mathbf{I} \cdot \tilde{x}_{i,k}$ is used to propagate the subintervals $i = \{\alpha, \beta\}$ to the following time-step.

5.1.2. Splitting of entries in modified system matrix

Alternatively, splitting of entries in the modified system matrix as in the 2D example

$$\tilde{x}_{\alpha,k} = \tilde{\mathbf{A}}_{\alpha,k-1}\tilde{x}_0 = \begin{bmatrix} a'_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \cdot \tilde{x}_0 \quad \text{and} \quad \tilde{x}_{\beta,k} = \tilde{\mathbf{A}}_{\beta,k-1}\tilde{x}_0 = \begin{bmatrix} a''_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \cdot \tilde{x}_0 \tag{5}$$

with $a'_{11} = [\underline{a}_{11}; \mathrm{mid}(a_{11})]$ and $a''_{11} = [\mathrm{mid}(a_{11}); \overline{a}_{11}]$ can be applied. After splitting, part of the information stored in the system matrix is still available. However, $\mathrm{int}\{x_{\alpha,k}\} \cap \mathrm{int}\{x_{\beta,k}\} \neq \emptyset$. The matrix entry i^*, j^* which has to be split is determined after normalization of the system matrix

$$\mathbf{S}^{(l)} = \mathrm{diag}(1./\mathrm{mid}(x_k^{(l)})) \cdot \mathbf{A}^{(l)} \cdot \mathrm{diag}(x_0^{(l)}) \tag{6}$$

for $l = 1, \ldots, \mathrm{length}\{L\{x_k\}\}$, where ./ denotes element-by-element division. After selection of the subinterval l^* according to

$$\max_{l=1,\ldots,\mathrm{length}\{L\{x_k\}\}} \left\{ \sum_{i,j} \mathrm{diam}(s_{i,j}^{(l)}) \right\} \to l^*, \tag{7}$$

where $\mathrm{diam}(\cdot)$ is the interval diameter, the matrix entry with the maximum diameter

$$\max_{i,j} \{\mathrm{diam}(s_{i,j}^{(l^*)})\} \to i^*, j^* \tag{8}$$

is chosen. Simulation is continued with $\tilde{x}_{i,k+1} = \mathbf{A}_k(x_{i,k})\tilde{\mathbf{A}}_{i,k-1}\tilde{x}_0$, $i = \{\alpha, \beta\}$.

5.2. Merging strategies and re-approximation by disjoint subintervals

To limit the number of interval boxes, merging of two subintervals $\tilde{x}_{i,k+1} = \tilde{\mathbf{A}}_{i,k}\tilde{x}_{i,0}$, $i = \{\alpha, \beta\}$, which can be replaced with small overestimation, is done by the conservative enclosure $\tilde{x}_{\alpha,k+1} \cup \tilde{x}_{\beta,k+1} \subseteq (\tilde{\mathbf{A}}_{\alpha,k} \cup \tilde{\mathbf{A}}_{\beta,k}) \cdot (\tilde{x}_{\alpha,0} \cup \tilde{x}_{\beta,0})$. The $\cup$-operator is applied element-wise for all matrix and vector entries.

Efficiency of splitting strategies decreases as soon as a huge number of significantly overlapping subintervals exist. Therefore, re-approximation by a conservative outer enclosure using disjoint subintervals is employed. Starting with

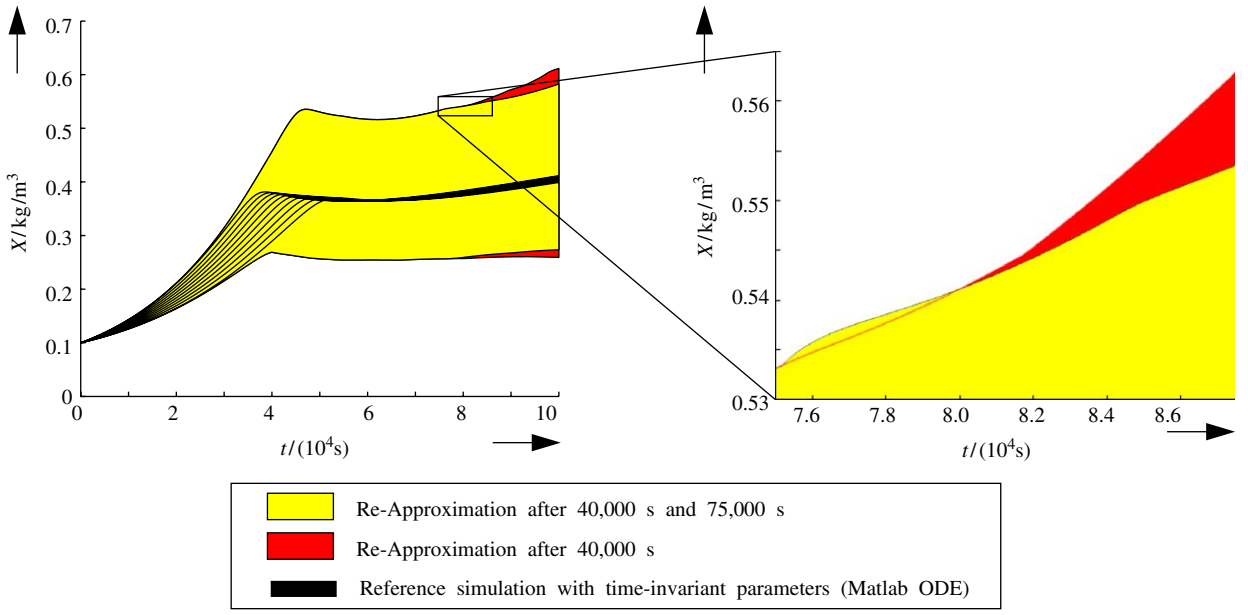

Fig. 4. Comparison of simulation results of the bacteria concentration X.

the hull of all subintervals (one interval box), splitting into subintervals in order to get a conservative approximation of the original overlapping interval boxes is performed. In the presented simulation results the stopping criterion was chosen as a desired number of interval boxes after re-approximation. As shown in the simulation result in Fig. 4, the simulation quality is improved after a short-time widening of the interval enclosures. Furthermore, in Fig. 4 the interval simulation is compared to a grid-based Matlab ODE simulation with different time-invariant values for $\hat{\mu}_{\mathrm{H}}$.

6. Conclusions and outlook on future research

In this paper, an efficient interval arithmetic simulation approach for the calculation of guaranteed enclosures of the state variables of biological wastewater treatment processes under consideration of interval uncertainties of the system parameters has been presented. The proposed splitting, merging, and re-approximation strategies improve the simulation quality significantly by better approximation of complex shaped regions in the state space. Together with a pseudo-linear transformation of the considered set of state equations they aim at the reduction of the wrapping effect. In future work, this algorithm is applied to optimization and robust controller design of nonlinear uncertain dynamical systems.

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